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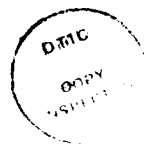
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)  <b>The technical content of this final report describes numerical methodology for analyzing a broad class of materials processing problems. The method emphasizes a close coupling of heat transfer, plastic deformation, and phase transformation. Implementation of the theoretical developments into a finite element calculation is discussed.</b>		

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Thermomechanical Analysis with Phase Transformations:  
A Unified Approach

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### Summary of Project

The major results of this research project are as follows: (1) A scheme was devised to model the physical phenomena of plastic deformation, heat transfer, and phase transformation in a unified way. (2) This scheme was incorporated into a finite element method so that physical problems involving the coupling of all three phenomena could be analyzed. (3) Calculations were performed for two prototype problems: quenching of a ball bearing and of a cylindrical Jominy specimen. (4) Two papers were written. The first is titled "Selective Reduced Integration for the Lagrangian Formulation," and it has been sent to ARO previously. The second has the same title as this research project and is included here as the main component of the final report.

Dr. Daniel C. Peirce was the principal investigator for this project. From time to time, he consulted with Dr. Peter D. Hilton and Dr. John L. O'Brien.

THERMOMECHANICAL ANALYSIS  
WITH  
PHASE TRANSFORMATIONS:  
A UNIFIED APPROACH

by Daniel C. Peirce

December 1988

## 1. Introduction.

Numerical modeling of materials processing has expanded considerably in recent years. Greater computing power and broader understanding of constitutive behavior have made finite element calculations of complex deformations both more practical and more accurate. In addition, heat transfer and other thermal effects are now routinely included in analyses of such processes as rolling and forging [1-3]. Models of quenching and heat treatment, however, have developed separately from efforts on processes involving materials forming [4-5], no doubt due to the relatively lesser roles of heat transfer and phase transformation in the latter, together with the relatively greater extent of plastic flow. The aim of this paper is to establish a modeling framework wherein the effects of heat transfer and phase change may be coupled with plastic deformation in a unified way. While specific attention here will be focused on examples of quenching procedures, the framework developed should broaden the capabilities of modeling for a wide range of materials processes.

A brief review of previous work which has proceeded in this direction indicates the need for the type of unifying approach that will be proposed here. Inoue and Raniecki [6] presented a table of research papers which had dealt with determination of quenching stresses, but only a few of the studies referenced in their table combined all three effects of phase change, thermal stress, and plasticity. Inoue and Raniecki built on these works to develop a careful treatment of the quenching problem, with special attention given to the plasticity formulation. Nevertheless, their analyses of the heat transfer and corresponding phase transformation history is completed prior to and independently of their solution of the plasticity problem (which predicts residual stresses).

Subsequent work by Sjöström [7] and Hildenwall and Ericsson [8] also included the effects of plastic flow, but the heat transfer and phase transformation calculation remained decoupled from the stress analysis. The studies by Fischer *et al* [9,10] kept the stress

analysis separate too, but they took special care to account for the temperature dependence of material properties for the heat transfer and phase change calculation. None of these methodologies, though, includes the effect of latent heat of transformation, heating due to plastic work, and the stress influence on phase changes. While these effects may be small in many situations, a flexible and unified approach should allow for their presence.

Inoue and Wang [11] recognized the completeness of this coupling which exists among heat transfer, phase change, and plastic flow. Denis *et al* [4] also took account of the stress effects on martensitic transformation, and emphasized their treatment of the transformation distortion as additional plastic strain. These papers provide careful analysis of the phase change and thermal effects, but these are coupled with the plastic flow by using a simple incremental approach in which the heat transfer and stiffness equations are solved in alternating fashion.

This incremental approach to coupled analysis has been used often for research on thermomechanical problems which do not involve phase transformations. For example, Dawson and his coworkers have developed finite element programs to model thermomechanical response in such applications as salt mines and forming of porous materials [12–14]. Chandra and Mukherjee [2] developed a coupled formulation for forming processes with heat transfer, and they used it to solve an extrusion problem. In contrast to these approaches, Rebelo and Kobayashi [1] developed a procedure for coupled analysis which employs an iterative scheme. The iterations serve to maintain close contact between the thermal and mechanical solutions. Absent from their constitutive equations, however, are elastic deformations; these are important in many situations, such as when an accurate determination of residual stresses is required.

The modeling framework presented here will attempt to bring together the best features of both the quenching and the metal forming research represented in the foregoing. The intent is not to give the final answer on which constitutive models and which phase

transformation laws are the correct ones for solving materials processing problems. Rather, the goal here is to formulate equations which are general enough to accommodate readily any or all of the key phenomena which occur in thermomechanical problems with phase changes. The pertinent aspects of these phenomena will be further discussed below, but reference is made here to the chart presented by Inoue and Wang [11] and reproduced with slight variation in Figure 1. This chart shows that temperature and stress affect each other, that stress and phase change affect each other, and that phase change and temperature affect each other. The equations to be developed here will be able to model all these interactions, and they will provide for great flexibility in the descriptions of plasticity and phase changes. The formulation established below has been applied to example problems of the quenching of a ball bearing and a Jominy end quench. The details of these and future applications are reserved for future reports.

## **2. Modeling Background.**

This section discusses large deformation mechanics, phase transformation, and heat transfer in turn. The separate models for these phenomena will provide the basis for the unified coupling to be described in Section 3.

**2.1 Large deformations and plasticity.** The ultimate use for the methodology proposed here is its incorporation into a finite element framework. In such a framework, incremental equilibrium is enforced by relying on the incremental principle of virtual work

$$\int_{V_0} \mathbf{t} \cdot \delta \mathbf{F} \, dV = \int_{S_0} \mathbf{T} \cdot \delta \mathbf{u} \, dS. \quad (2.1)$$

Here, the nominal stress  $\mathbf{t}$  and deformation gradient  $\mathbf{F}$  are calculated with respect to the reference configuration, which has volume  $V_0$  and surface  $S_0$ . In many cases, the reference configuration corresponds to the initial undeformed state of the body. The vector

$\mathbf{T}$  is the nominal traction vector, and  $\mathbf{u}$  is the displacement vector. Constitutive relations are often expressed conveniently in terms of the Kirchhoff stress  $\boldsymbol{\tau}$ , which is related to the nominal stress  $\mathbf{t}$  and Cauchy stress  $\boldsymbol{\sigma}$  by

$$\boldsymbol{\tau} = \mathbf{F} \cdot \mathbf{t} = J\boldsymbol{\sigma}, \quad (2.2)$$

where  $J$ , the Jacobian of the deformation, is the determinant of  $\mathbf{F}$ .

For material models which incorporate elastic behavior, incremental response is based on the relationship

$$\dot{\boldsymbol{\tau}} = \mathbf{L} : \mathbf{D}^e, \quad (2.3)$$

where  $\dot{\boldsymbol{\tau}}$  is the Jaumann rate of Kirchhoff stress,  $\mathbf{L}$  is the tensor of elastic moduli, and  $\mathbf{D}^e$  is the elastic portion of the deformation rate tensor  $\mathbf{D}$ , which is the symmetric part of  $\mathbf{F} \cdot \mathbf{F}^{-1}$ . Further details of the Jaumann rate and the kinematics behind equation (2.3) may be had from a variety of sources, including Needleman [15,16] and Anand *et al* [17]. For the kinds of problems under consideration here, the deformation rate  $\mathbf{D}$  is made up of several distinct constituents in addition to  $\mathbf{D}^e$ :

$$\mathbf{D} = \mathbf{D}^e + \mathbf{D}^{vp} + \mathbf{D}^{tr} + \mathbf{D}^{te}, \quad (2.4)$$

where  $\mathbf{D}^{vp}$  represents the contribution from viscoplasticity,  $\mathbf{D}^{tr}$  contains the effects of phase transformation, and  $\mathbf{D}^{te}$  incorporates the influence of thermal expansion and contraction. Each of these terms must be expressed in such a way that (2.3) may be inserted into (2.1) and stiffness equations derived. This subsection focuses on  $\mathbf{D}^{vp}$ , while  $\mathbf{D}^{tr}$  and  $\mathbf{D}^{te}$  will be discussed in connection with phase transformation and heat transfer, respectively.



A viscoplastic formulation is used here because strain-rate dependence and creep play important roles in many materials processes. With some loss of generality, attention will be restricted to materials which harden isotropically, and for which the plastic deformation rate  $D^{vp}$  is always aligned with the Kirchhoff stress deviator  $\mathbf{s}$ . For rate-independent materials, these assumptions are consistent with  $J_2$  flow theory. Potential variations from these restrictions include pressure-sensitive plastic flow and kinematic hardening behavior. (Indeed, the former will play a role here due to equation (2.10) introduced later.) There is no reason that such behavior cannot be included in what follows, and reference is made to Anand *et al* [17] and Peirce *et al* [18], where further details on modeling these and other effects may be found. The presentation here, however, becomes involved enough even with the various assumptions put forth above.

The Kirchhoff stress deviator and related quantities are defined as follows:

$$\mathbf{s} \equiv \boldsymbol{\tau} - \frac{1}{3}(\mathbf{I} : \boldsymbol{\tau}) \mathbf{I}, \quad \tau_e^2 \equiv \frac{3}{2} \mathbf{s} : \mathbf{s}, \quad (2.5a)$$

$$\mathbf{p} \equiv \frac{3\mathbf{s}}{2\tau_e}, \quad \mathbf{P} \equiv \mathbf{L} : \mathbf{p}. \quad (2.5b)$$

Here  $\tau_e$  represents the effective Kirchhoff stress, and  $\mathbf{p}$  and  $\mathbf{P}$  are tensors which prove convenient in the subsequent development. It follows from (2.5b) that  $\mathbf{p} : \mathbf{p} = 3/2$ . The viscoplastic deformation rate may now be written

$$D^{vp} = \dot{\epsilon}^{vp} \mathbf{p}, \quad (2.6)$$

where the accumulated viscoplastic strain  $\epsilon^{vp}$  is defined as

$$\epsilon^{vp} \equiv \int_0^t \dot{\epsilon}^{vp} dt' = \int_0^t \left( \frac{2}{3} D^{vp} : D^{vp} \right)^{\frac{1}{2}} dt'. \quad (2.7)$$

A tremendous research effort has been expended on determination of useful functional forms for  $\dot{\epsilon}^{vp}$ , which may in general depend on stress, temperature, plastic work, and several state variables. Here again, attention will be restricted to a limited subset of the general case, to be represented as follows:

$$\dot{\epsilon}^{vp} = f(\tau_e, \epsilon^{vp}, T, p_i), \quad (2.8)$$

where  $T$  is temperature, and each  $p_i$  here represents the volume fraction of phase  $i$  of the material. The development which follows could be carried out equally well with different choices for (2.8); examples include the models proposed by Merzer and Bodner [19] and Anand [20].

At this point, the form (2.6) with (2.8) specified is enough to provide the plasticity input to the incremental virtual work principle (2.1). The functional expressions typically associated with (2.8) give rise to stiff response when time integration is attempted. Moderation of this stiff behavior is a key reason for the development of the integration techniques to be developed in Section 3.

**2.2 Phase transformations.** The distortion induced by a phase transformation, represented here by  $D^{tr}$ , arises from volume changes associated with the growth of a new phase. The volume increase which typically accompanies a martensitic transformation is an excellent example of this phenomenon. The magnitudes of such volume changes are generally well-characterized, and will be denoted here by  $3b_i$ , on a percentage basis, for appearance of each phase  $i$ . Therefore,

$$D^{tr} = I \sum_i b_i \dot{p}_i. \quad (2.9)$$

The analogy between  $b_i$  and the coefficient of thermal expansion is worth noting. to be completely general, it would be better to write (2.9) with two subscripts on each character

to correspond to a specific transformation (from phase  $i$  to phase  $j$ , say). It is often the case, however, that a specific phase is formed in only one way; in addition, the number of phases worth considering in many applications will likely be three or fewer, so that (2.9) should not be the source of any confusion.

While accurate values for  $b_i$  are generally quite accessible, the nucleation and growth of a new phase can proceed in any number of ways, and suitably realistic models for the evolution of the phases  $p_i$  are complex. For the purposes of this work, it will be assumed that the  $p_i$  may be represented in functional form as

$$p_i = p_i(\tau_e, \tau_h, T, t), \quad (2.10)$$

where  $T$  is temperature and  $t$  is time; of course, the  $p_i$  must sum to unity. The effective stress  $\tau_e$  has been defined in (2.5a), while  $\tau_h$  is roughly thrice the negative pressure  $-p$ , that is

$$\tau_h \equiv I : \tau = J(I : \sigma) = -3pJ. \quad (2.11)$$

Although situations no doubt exist where (2.10) is too restrictive, such as when chemistry or grain size come into play, these factors are usually fixed during a given process. Equation (2.10) does account for some of the key driving forces for phase changes: stress, temperature, and time.

The transformation of austenite to pearlite and martensite during quenching of steel furnishes a useful example of possible choices for specification of (2.10). These phases will be denoted here by  $p_a$ ,  $p_p$ , and  $p_m$  respectively, with  $p_a = 1 - p_p - p_m$ . For pearlitic growth, an equation along the lines of the sigmoidal curve proposed by Johnson and Mehl [21] may be used:

$$p_p = 1 - \exp[-a(T)t^n]. \quad (2.12)$$

The form of  $a(T)$  depends on the nucleation and growth rates in the material at hand, but its explicit variation with temperature  $T$  allows it to account for the knee in the time-temperature-transformation curve. The exponent  $n$  is related to the shape of the growing phase. More detailed possibilities for (2.12) are discussed at length by Inoue and Raniecki [6]. For the martensite transformation, an expression of the form

$$p_m = (1 - p_p) \left\{ 1 - \exp[\phi(T - M_s)] \right\}, \quad (2.13)$$

valid only when  $T$  is less than the martensite start temperature  $M_s$ , is discussed by Inoue and Raniecki [6] and Hakberg and Högborg [5], among many others. The parameter  $\phi$  is presumed constant here.

Equations (2.12) and (2.13) show no dependence on stress, but this may be introduced easily by allowing  $a(T)$  or  $M_s$  to change with pressure or effective stress. Because formation of martensite results in an instantaneous volume increase, the  $M_s$  temperature is effectively increased under hydrostatic tension, and decreased under hydrostatic pressure. This kind of effect may be easily incorporated in (2.13). While particular cases may require greater detail than is contained in the above expressions for pearlite and martensite growth, the latter nevertheless indicate how key aspects of these phase transformations may be modeled.

**2.3 Heat transfer.** The first role of heat transfer is to drive thermal stresses via  $D^{te}$  in (2.4). Under the assumption that each phase  $p_i$  has a coefficient of thermal expansion  $\alpha_i$ , a reasonable approximation is

$$D^{te} = I \left( \sum_i \alpha_i p_i \right) \dot{T}. \quad (2.14)$$

If appropriate, more accurate expressions for the coefficient of thermal expansion, parenthesized in (2.14), may be found in Bobeth and Diener [22] and Hashin [23]. Temperature also has influence by its effect on viscoplasticity, as in (2.8), and especially on phase transformation, as in (2.12) and (2.13). In addition, many material properties, including elastic moduli, coefficients of thermal expansion, and the thermal properties to be introduced in this section, may vary significantly with temperature.

For all these reasons, the heat transfer equation must be solved, together with the equilibrium equation (2.1), to provide a complete description of many materials processes. The form of the heat transfer equation employed here is

$$\rho c_p \dot{T} = \nabla \cdot (\kappa \nabla T) + q, \quad (2.15)$$

where  $\rho$  is the material density,  $c_p$  is the specific heat,  $\kappa$  is thermal conductivity, and  $q$  represents all heat source terms. For multiphase materials in which the phases have different thermal properties, weighted averages of these properties may be substituted in (2.15) if the property variations among the phases are not too great. Because equation (2.15) will be used to model heat flow in a deforming material, the meaning of the gradient must be considered carefully. As discussed by Lemonds and Needleman [24], heat conduction depends at root on the spacing between atoms, which is not affected by plasticity, but only by elastic straining. Therefore, if the gradient in (2.15) is taken with respect to the reference configuration, the error incurred will be of the order of the elastic strains, which are typically much less than one percent. Adjustment of the gradient with respect to the elastic deformation may be performed if this additional accuracy is needed, but in a numerical calculation, substantial extra work associated with splitting the deformation gradient would be required. If significant changes in atom spacing are associated with phase transformation, they are perhaps best handled through adjustment

of the thermal conductivity  $\kappa_i$  associated with the particular phase.

Further influence of the deforming material on (2.15) is felt through the source terms  $q$ . In the present development, these source terms will include the heating due to plastic working and the latent heat of transformation:

$$q = \chi \tau : D^v p + \sum_i (\rho h)_i p_i. \quad (2.16)$$

In this equation, the parameter  $\chi$ , which represents the fraction of plastic work which actually contributes to a temperature rise in the body, was used by Lemonds and Needleman [24]. When one phase is transformed into another phase  $p_i$ , the latent heat is denoted here by  $h_i$ , expressed as energy per unit mass of transformation product. With the corresponding density  $\rho_i$ ,  $(\rho h)_i$  represents the latent heat per unit volume of newly produced phase  $i$ . The same remarks about two subscripts which were made in connection with (2.9) also apply to (2.16), but, at the risk of some confusion, the single subscript is used for brevity.

It is clear from equations (2.4) and (2.15) and their ingredients that the thermal and mechanical responses of many materials processes are inseparably coupled. For solution of these equations, a numerical approach which reflects this coupling therefore has great appeal. The methodology to be developed here attempts to exploit the interdependence of the relevant field quantities in an incremental scheme which follows the true evolution of these quantities accurately. In addition, maintaining the closeness of the coupling throughout the numerical approach reduces the tendency to instability and may allow significantly larger time increments to be used.

### 3. Numerical method.

Even with the various special assumptions made throughout Section 2, there remains a great deal of complexity in the models of the physical phenomena discussed.

This section therefore begins with a summary presentation of the final numerical scheme, with description of its full detail and derivation to follow.

**3.1 Coupling of the mechanical and thermal solutions.** As noted in Section 2, the mechanical response is kept in equilibrium by the incremental virtual work principle (2.1). The method for implementing (2.3) in (2.1) may be found elsewhere [15,16]. The key task for modeling the mechanical response is thus to specify (2.3) in detail. As subsequent manipulations will show, the Jaumann rate of Kirchhoff stress takes the form

$$\dot{\tau} = C : D + G_5 P + G_6 I + (G_7 P + G_8 I) \dot{T}, \quad (3.1)$$

where  $G_k \equiv N^{-1}H_k$ ,  $C$  is given by

$$C = N^{-1}[L - H_1 P P - H_2 P I - H_3 I P - H_4 I I], \quad (3.2)$$

and  $N$  and the  $H_k$  for  $k = 1$  to  $8$  are defined later. At this point, it should be noted that (3.1) depends on deformation rate  $D$ , temperature rate  $\dot{T}$ , and the other terms in the middle of the right-hand side, which may be specified completely in terms of the current state. These terms are analogous to the residual loading terms which appear in many plasticity formulations. In (3.2), unless  $H_2 = H_3$ , the moduli  $C$  do not lead to a symmetric stiffness matrix in a finite element formulation. This aberration arises quite expectedly from the stress dependence of the phase transformations as indicated in (2.10). It will be seen later that if stresses do not appear in (2.10),  $H_2 = H_3 = 0$ .

Treatment of the heat transfer equation by finite elements requires that (2.15) be multiplied by a variation in temperature  $\delta T$  and integrated over a reference volume. As in [24], this results in

$$\int_{V_0} \rho c_p \dot{T} \delta T dV = - \int_{V_0} \kappa (\nabla T) \cdot (\nabla \delta T) dV + \int_{V_0} q \delta T dV + \int_{S_0} \kappa (\mathbf{n} \cdot \nabla T) \delta T dS. \quad (3.3)$$

Here,  $\mathbf{n}$  is the unit outward normal to the body in the reference configuration. Equation (3.3) leads to the following equations for the nodal temperatures  $T_j$  and their rates  $\dot{T}_j$  [24]:

$$M_{ij} \dot{T}_j + D_{ij} T_j = Q_i. \quad (3.4)$$

Here, the subscripts  $i$  and  $j$  refer to finite element nodes and the matrices represented by  $M_{ij}$  and  $D_{ij}$  are derived in standard fashion from the integrals in (3.3). The following approach is adopted here for the solution of (3.4). For some  $\theta$ ,  $0 \leq \theta \leq 1$ , equation (3.4) is presumed to hold at time  $t + \theta\Delta t$ , where  $t$  is the time and  $\Delta t$  is the time increment. The value of  $T_j$  at  $t + \theta\Delta t$  is linearly interpolated from its values at  $t$  and  $t + \Delta t$ . As a result, the equation may be multiplied by  $\Delta t$  and rearranged to give

$$(M_{ij} + \theta\Delta t D_{ij}) T_j(t + \Delta t) = (M_{ij} - (1 - \theta)\Delta t D_{ij}) T_j(t) + Q_i(t + \theta\Delta t), \quad (3.5)$$

which may readily be solved for  $T_j(t + \Delta t)$ . The nodal values  $Q_i(t + \theta\Delta t)$  arise from (2.16) and depend on any source terms that may be present as well as on the current increment of mechanical behavior through the plastic work increment derived later in (3.14).

Equation (3.4) in turn is coupled with the mechanical equilibrium equations for the nodal displacement rates  $\dot{U}_j$ :



$$K_{ij} \dot{U}_j + C_{ij} \dot{T}_j = F_i. \quad (3.6)$$

The finite element matrices  $K_{ij}$  and  $C_{ij}$  are derived from inserting (3.1) into (2.1). Both (3.4) and (3.6) depend on increments of both the nodal temperatures and the nodal displacements; the latter enter (3.4) via the vector of source terms  $Q_i$  which derive from (2.16).

The solution espoused here for the solution of the coupled equations (3.4) and (3.6) is somewhat similar to that put forth by Lemonds and Needleman [24]. At a particular time  $t$ , it is assumed that the current state is known and that the incremental fields  $\dot{T}_j$  and  $\dot{U}_j$  must be determined. First, an estimate of the temperature increments  $\dot{T}_j$  is obtained as follows. At each nodal point, a quadratic is fit to the values of  $T_j$  at the current time  $t$  and the two previous time steps. This quadratic is used to obtain a value of each  $T_j$  at time  $t + \Delta t$ , from which the temperature increment may be obtained by subtracting  $T_j(t)$ . With these estimates of the  $\dot{T}_j$ , equation (3.6) may be solved for the  $\dot{U}_j$ . This solution in turn provides the information required to specify  $Q_i(t + \theta\Delta t)$  and to solve (3.4) for a presumably more accurate set of the  $\dot{T}_j$ . This new set may be compared with the estimates from the quadratic fit, and if the difference is higher than a prescribed tolerance, an iterative procedure may be undertaken, or, as is the case with current applications of this approach, the entire increment may be recalculated with a smaller time step. To initialize a calculation, when previous temperature data are unavailable, it seems best to solve (3.4) without taking account of the mechanical behavior inputs to  $Q_i$ ; here again, the estimates thus arrived at can be checked once (3.6) has been solved and (3.4) solved again with the new information. The main drawback of repeated solutions of (3.4) is that they are much more expensive than quadratic fits. In quenching processes and other situations involving steep temperature gradients, however, a quadratic fit tends to

be less accurate than direct solution of (3.4) without the complete  $Q_i$ , because the rapid heat conduction dominates what is typically a smaller influence from the heat source terms.

Once the incremental fields  $\dot{U}_j$  and  $\dot{T}_j$  have been obtained from (3.4) and (3.6), the stresses, phases, and other internal variables may be updated. Finally, the displacements  $U_j$  and temperatures  $T_j$  at time  $t + \Delta t$  are calculated. At this point,  $t + \Delta t$  becomes the current time, and the next increment may begin.

**3.2 Derivation of the constitutive laws.** It remains to fill in the details of (3.1) and (3.2). The starting point is the viscoplastic deformation rate  $D^{vp}$  in equations (2.4) and (2.6). Because typical forms for (2.8) lead to stiff constitutive equations, the tangent modulus method proposed by Peirce, Shih, and Needleman [18] and extended by Anand *et al* [17] is followed in the present development in order to alleviate problems associated with the stiff equations. The tangent modulus method begins with the following frequently employed expression for  $D^{vp}$  in the middle of a time step:

$$\bar{D}^{vp} = (1 - \theta) D^{vp}(t) + \theta D^{vp}(t + \Delta t). \quad (3.7)$$

A simple expansion of (2.6) from the current time  $t$  is used to arrive at the approximation

$$\bar{D}^{vp} = (f + \theta \Delta f) \mathbf{p} + f \theta \Delta t \dot{\mathbf{p}}, \quad (3.8)$$

where  $\Delta f$ , by virtue of (2.8), is

$$\Delta f = \frac{\partial f}{\partial \tau_e} \Delta \tau_e + \frac{\partial f}{\partial \epsilon^{vp}} \Delta \epsilon^{vp} + \frac{\partial f}{\partial T} \Delta T + \sum_i \frac{\partial f}{\partial p_i} \Delta p_i, \quad (3.9)$$

and  $\dot{\mathbf{p}}$  may be determined from (2.5b):

$$\frac{\dot{\mathbf{v}}}{\mathbf{p}} = \frac{3\dot{\gamma}}{2\tau_e} - \frac{3\dot{\gamma}_h}{2\tau_e} \mathbf{I} - \frac{\mathbf{p}}{\tau_e} \dot{\gamma}_e. \quad (3.10)$$

Anand *et al* [17] included a term corresponding to the rightmost term in (3.8) to account for the change in direction of plastic flow during a time increment, and this has the added benefit of improving the ability of the scheme to follow nonproportional loading accurately. Note that when  $\dot{\mathbf{v}}$  is parallel to  $\mathbf{s}$  and hence to  $\mathbf{p}$ , the expression for  $\frac{\dot{\mathbf{v}}}{\mathbf{p}}$  in (3.10) vanishes.

The next step is expression of (3.9) in such a way that stress and phase increments are eliminated. From (2.5a) and (2.3), there follows

$$\Delta\tau_e = \mathbf{P} : \mathbf{D} \Delta t - \mathbf{P} : \mathbf{p} \Delta\epsilon^{vp}, \quad (3.11)$$

while (2.10) leads to

$$\Delta p_i = \frac{\partial p_i}{\partial \tau_e} \Delta\tau_e + \frac{\partial p_i}{\partial \tau_h} \Delta\tau_h + \frac{\partial p_i}{\partial T} \Delta T + \frac{\partial p_i}{\partial t} \Delta t. \quad (3.12)$$

Unfortunately, equation (3.12) introduces the additional quantity  $\Delta\tau_h$ , and this in turn requires that attention be shifted to  $\mathbf{D}^{tr}$  and  $\mathbf{D}^{te}$  in (2.10) and (2.14). Equations (2.3) and (2.4) lead to

$$\begin{aligned} \Delta\tau_h &= \mathbf{I} : \dot{\gamma} \Delta t = \\ &\mathbf{I} : \mathbf{L} : (\mathbf{D} \Delta t - \mathbf{I} \sum_i b_i \Delta p_i - \mathbf{I} (\sum_i \alpha_i p_i) \Delta T). \end{aligned} \quad (3.13)$$

After the identification  $\Delta\epsilon^{vp} = (f + \theta\Delta f) \Delta t$  has been made, simultaneous solution of (3.9) and (3.11) through (3.13) is required to determine expressions for the incremental quantities above in terms of just  $\Delta t$ ,  $\mathbf{D}\Delta t$ , and  $\Delta T$ . The algebra involved in carrying

out this solution is quite cumbersome. The details are made more tractable by using (3.12) only after it has been summed against the phase change expansion coefficients  $b_i$ , and by seeking expressions for incremental scalar quantities that represent sums of four terms, each of which involves  $\Delta t$ ,  $P:D \Delta t$ ,  $I:D \Delta t$ , and  $\Delta T$ . The procedure is not unlike that employed to invert Hooke's law when using index notation. The key results of these manipulations may be summarized as follows:

$$(f + \theta \Delta f) \Delta t = F_1 \Delta t + F_2 P:D \Delta t + F_3 I:D \Delta t + F_4 \Delta T, \quad (3.14)$$

$$\sum_i b_i \Delta p_i = B_1 \Delta t + B_2 P:D \Delta t + B_3 I:D \Delta t + B_4 \Delta T. \quad (3.15)$$

For simplicity, the assumption made here and from henceforth is that the elastic moduli are isotropic, and that they are specified by a bulk modulus  $\bar{\kappa}$  and shear modulus  $\mu$ . On this basis, the expressions for  $F_1$  through  $F_4$  are given by

$$F_1 = \beta [f + \theta \Delta t (A_1 - 9\bar{\kappa}\gamma A_3 R_1)] \quad (3.16a)$$

$$F_2 = \beta [\theta \Delta t (A_2 - 9\bar{\kappa}\gamma A_3 R_2)] \quad (3.16b)$$

$$F_3 = \beta [\theta \Delta t (3\bar{\kappa}\gamma A_3)] \quad (3.16c)$$

$$F_4 = \beta [\theta \Delta t (A_4 - 9\bar{\kappa}\gamma A_3 (R_4 + \sum_i \alpha_i p_i))], \quad (3.16d)$$

where

$$\beta = [1 + \theta \Delta t (3\mu A_2 - A_5 - 27\bar{\kappa}\mu\gamma A_3 R_2)]^{-1}, \quad (3.17)$$

$$\gamma = [1 + 9\bar{\kappa} \sum_i b_i \frac{\partial p_i}{\partial \tau_h}]^{-1}, \quad (3.18)$$

and  $A_1$  through  $A_5$  are given by

$$A_1 = \sum_i \frac{\partial f}{\partial p_i} \frac{\partial p_i}{\partial t}, \quad (3.19a)$$

$$A_2 = \frac{\partial f}{\partial \tau_e} + \sum_i \frac{\partial f}{\partial p_i} \frac{\partial p_i}{\partial \tau_e}, \quad (3.19b)$$

$$A_3 = \sum_i \frac{\partial f}{\partial p_i} \frac{\partial p_i}{\partial \tau_h}, \quad (3.19c)$$

$$A_4 = \frac{\partial f}{\partial \Gamma} + \sum_i \frac{\partial f}{\partial p_i} \frac{\partial p_i}{\partial \Gamma}, \quad (3.19d)$$

$$A_5 = \frac{\partial f}{\partial \epsilon_{vp}}. \quad (3.19e)$$

Further, the definitions of  $R_1$  through  $R_4$  are

$$\begin{aligned} R_1 &= \sum_i b_i \frac{\partial p_i}{\partial t}, & R_2 &= \sum_i b_i \frac{\partial p_i}{\partial \tau_e}, \\ R_3 &= \sum_i b_i \frac{\partial p_i}{\partial \tau_h}, & R_4 &= \sum_i b_i \frac{\partial p_i}{\partial \Gamma}. \end{aligned} \quad (3.20)$$

These allow  $B_1$  through  $B_4$  to be written as

$$B_1 = \gamma (R_1 - 3\mu F_1 R_2), \quad (3.21a)$$

$$B_2 = \gamma (R_2 - 3\mu F_2 R_2), \quad (3.21b)$$

$$B_3 = \gamma (3\bar{\kappa} R_3 - 3\mu F_3 R_2), \quad (3.21c)$$

$$B_4 = \gamma (R_4 - 3\mu F_4 R_2 - 9\bar{\kappa} R_3 \sum_i \alpha_i p_i). \quad (3.21d)$$

Finally, the details of (3.1) and (3.2) may be filled in. The definition of  $N$  may be recognized relatively easily from (3.8) and (3.10):

$$N \equiv 1 + \frac{3\mu f \theta \Delta t}{\tau_e} \quad (3.22)$$

The definitions of  $H_1$  through  $H_8$  are as follows:

$$H_1 \equiv NF_2 - \frac{f\theta\Delta t}{\tau_e} \quad (3.23a)$$

$$H_2 \equiv NF_3 \quad (3.23b)$$

$$H_3 \equiv 3\bar{\kappa}B_2N \quad (3.23c)$$

$$H_4 \equiv 3\bar{\kappa}B_3N - \frac{3\bar{\kappa}\mu f\theta\Delta t}{\tau_e} \quad (3.23d)$$

$$H_5 \equiv -NF_1 \quad (3.23e)$$

$$H_6 \equiv -3\bar{\kappa}B_1N \quad (3.23f)$$

$$H_7 \equiv -NF_4 \quad (3.23g)$$

$$H_8 \equiv -3\bar{\kappa}(B_4 + \Sigma\alpha_i p_i) N \quad (3.23h)$$

These equations, while cumbersome, specify the constitutive law (3.1) completely.

Several assumptions have been made during this derivation, but there are also several key effects which have not been written off. For example, the important influences of pressure on phase changes has been included; this is reflected in the lack of symmetry of the moduli  $C$  in (3.2). The complexity of equations (3.16) to (3.23) may be collapsed considerably if additional assumptions are made with respect to equations (2.8) or (2.10). If more generality is needed than these equations afford, the manipulations summarized above may be redone in similar fashion to obtain appropriate parallels to (3.23).

**4. Conclusion and Future Work.** Perhaps the primary impetus for development of the modeling procedures described above is the need for solutions to problems which occur during quenching processes, such as adverse residual stresses and quench cracking. It is during such processes that phase transformations join thermomechanical response as key features of the material behavior. But phase changes play important roles in other processes as well, and they may be driven more by deformation than by temperature in bulk forming processes like rolling and forging. The methodology described above can easily be simplified or enhanced depending on the important parameters in a particular problem. For example, the temperature dependence of elastic moduli may play a key role

in many processing problems; even though such dependence has not been included here, it is typically smooth and may be easily incorporated into the formulation.

The initial application of the work in this manuscript uses the present methodology to analyze two quenching problems: a ball bearing and an end quench. The ball bearing problem was analyzed using a simplified version of the procedure discussed above. In particular, the mechanical effects on the heat conduction behavior were neglected so that the thermal response was independent of the mechanical and phase responses, which were coupled. The end quench problem did not make these simplifications, as it included all the coupling effects described in the foregoing analysis. The computations performed for these two quenching problems illustrated some important considerations for conducting such numerical calculations, especially those in which high gradients are involved, and these will be discussed in subsequent work. Beyond the solution of these sample problems, it is anticipated that the present work will soon find practical application to the solution of processing problems in gun barrel quenching.

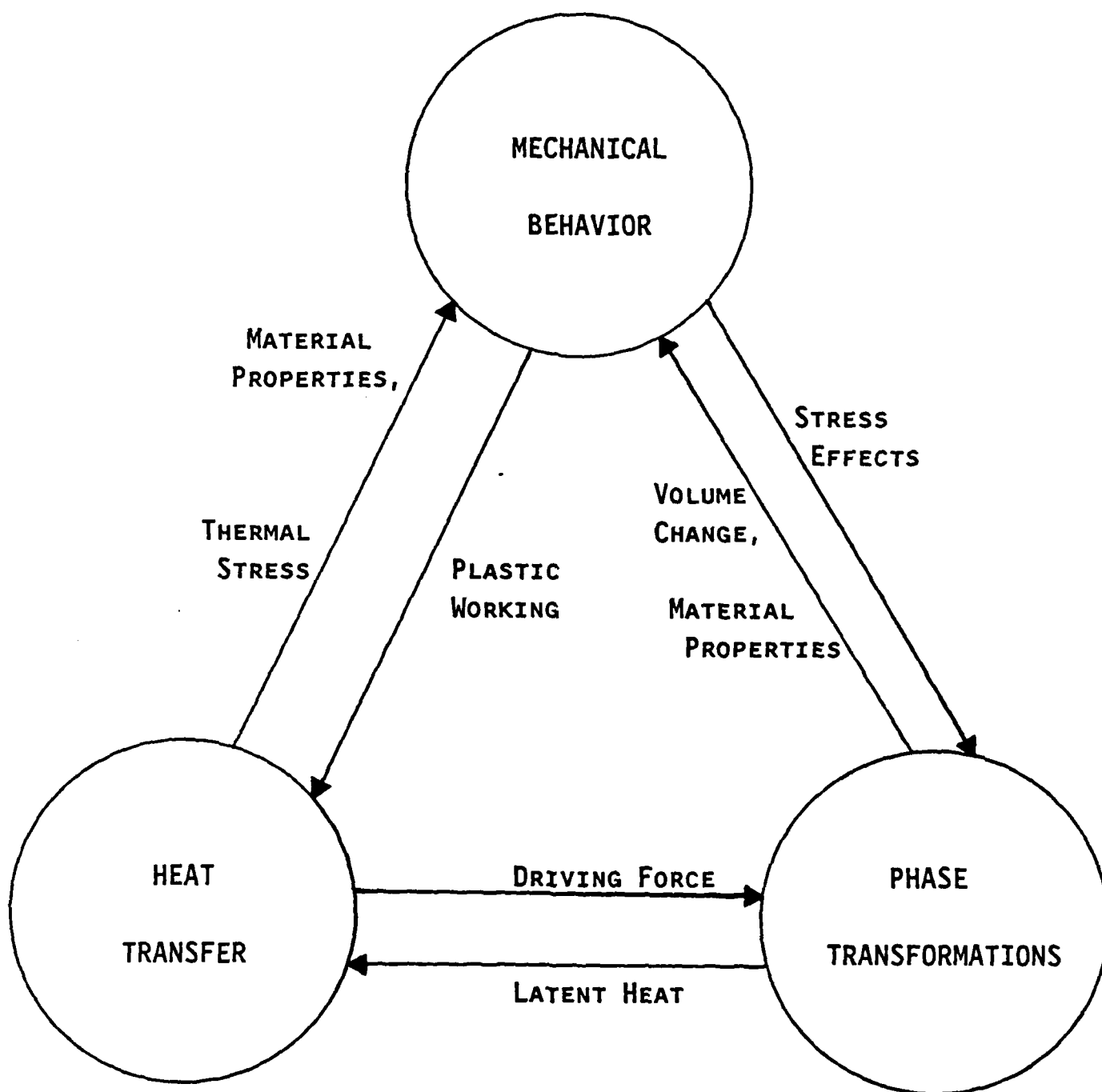


FIGURE 1

This schematic indicates the key coupling mechanisms in materials processing problems.



## REFERENCES

- [1] N. Rebelo and S. Kobayashi, *A Coupled Analysis of Viscoplastic Deformation and Heat Transfer – I*, Int. J. Mech. Sci. **22** 699–705 (1980).
- [2] A. Chandra and S. Mukherjee, *A Finite Element Analysis of Metal Forming Processes with Thermomechanical Coupling*, Int. J. Mech. Sci. **26** 661–676 (1984).
- [3] J. T. Oden, D. R. Bhandari, G. Yagawa, and T. J. Chung, *A New Approach to the Finite-Element Formulation and Solution of a Class of Problems in Coupled Thermoelastoviscoplasticity of Crystalline Solids*, Nuclear Engineering and Design **24** 420–430 (1973).
- [4] S. Denis, A. Simon, and G. Beck, *Analysis of the Thermomechanical Behavior of Steel During Martensitic Quenching and Calculation of Internal Stresses*, in Heat Treatment Shanghai 1983, Third International Congress on Heat Treatment of Materials, November 7–11, 1983.
- [5] B. Hakberg and T. Högborg, *A Mathematical Model for Hardening of Steel*, Materials Science and Engineering **35** 205–211 (1978).
- [6] T. Inoue and B. Raniecki, *Determination of Thermal Hardening Stress in Steels by Use of Thermal Plasticity Theory*, J. Mech. Phys. Solids **26** 187–212 (1978).
- [7] S. Sjöström, *Computer-Based Models for Quenching*, in Computers in Materials Technology, Proceedings of the International Conference at Linköping University,

Sweden, June 4–5, 1980, Pergamon Press 1981.

[8] B. Hildenwall and T. Ericsson, *How, Why, and When Will the Computed Quench Simulation Be Useful for Steel Heat Treaters?* in Computers in Materials Technology, Proceedings of the International Conference at Linköping University, Sweden, June 4–5, 1980, Pergamon Press 1981.

[9] D. F. Fischer, O. Gründler, W. Mitter, F. G. Rammerstorfer, and E. T. Till, *The Influence of Creep and Transformation Plasticity in the Analysis of Stresses Due to Heat Treatment*, in Numerical Methods in Thermal Problems, Volume 2, Proceedings of Conference in Venice, Italy, July 1981.

[10] F. G. Rammerstorfer, D. F. Fischer, W. Mitter, K. J. Bathe, and M. J. Snyder, *On Thermo-elastic-plastic Analysis of Heat-Treatment Processes Including Creep and Phase Changes*, *Computers & Structures* **13** 771–779 (1981).

[11] T. Inoue and Z. Wang, *Finite Element Analysis of Coupled Thermoelastic Problem with Phase Transformation*, in Numerical Methods in Industrial Forming Processes, Proceedings of the International Conference on Numerical Methods in Industrial Forming Processes, Swansea UK, July 12–16 1982. Pineridge Press.

[12] P. R. Dawson and D. E. Munson, *Numerical Simulation of Creep Deformations Around a Room in a Deep Potash Mine*, *Int. J. Rock Mech. Min. Sci. and Geomech.* **20** 33–42 (1983).

[13] J. R. Tillerson and P. R. Dawson, *Heated Mine Room and Pillar Secondary Creep Response*, *International Journal for Numerical and Analytical Methods In Geomechanics* **5**

177–193 (1981).

[14] P. R. Dawson, *A Model for Analyzing the Forming of Porous Materials*, in proceedings of The Application of Numerical Methods to Manufacturing Processes Symposium, 1983 ASM Metals Congress, ASM Paper 8305–029 (1983).

[15] A. Needleman, *Finite Elements for Finite Strain Plasticity Problems*, in Plasticity of Metals at Finite Strain, E. H. Lee and R. H. Mallett, eds., pp. 387–436 (1982) Stanford University.

[16] A. Needleman, *On Finite Element Formulations for Large Elastic–Plastic Deformations*, presented at the Symposium on Advances and Trends in Structures and Dynamics, October 1984.

[17] L. Anand, A. Lush, M. F. Briceno, and D. M. Parks, *A Time–Integration Procedure for a Set of Internal Variable Type Elasto–Viscoplastic Constitutive Equations*, Department of Mechanical Engineering Report, Massachusetts Institute of Technology, September 1985.

[18] D. Peirce, C. F. Shih, and A. Needleman, *A Tangent Modulus Method for Rate Dependent Solids*, Computers & Structures 18 875–887 (1984).

[19] A. Merzer and S. R. Bodner, *Analytical Formulation of a Rate and Temperature Dependent Stress–Strain Relation*, Transactions of the ASME Journal of Engineering Materials and Technology 101 254–257 (1979).

[20] L. Anand, *Constitutive Equations for the Rate Dependent Deformation of Metals at*

*Elevated Temperatures*, Transactions of the ASME Journal of Engineering Materials and Technology **104** 12–17 (1982).

[21] W. A. Johnson and R. F. Mehl, Transactions of the AIME **135** p. 416 (1939).

[22] M. Bobeth and G. Diener, *Static Elastic and Thermoelastic Field Fluctuations in Multiphase Composites*, J. Mech. Phys. Solids **35** 137–149 (1987).

[23] Z. Hashin, *Thermal Expansion of Polycrystalline Aggregates, I and II*, J. Mech. Phys. Solids **32** 149–165 (1984).

[24] J. LeMonds and A. Needleman, *Finite Element Analyses of Shear Localization in Rate and Temperature Dependent Solids*, Mechanics of Materials **5** 339–362 (1986).